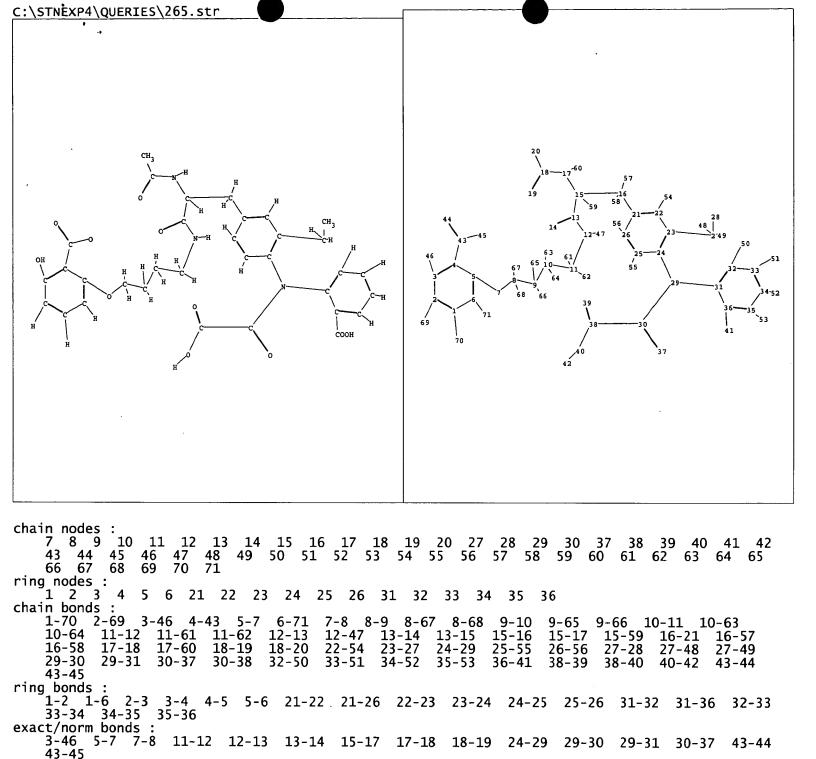
$2-\{4-[(N-acetyl-4-[(carboxycarbonyl)(2-carboxyphenyl)amino]-3-ethylphenylalanyl)amino]butoxy$ 

2-{4-[(N-acetyl-4-[(carboxycarbonyl)(2-carboxyphenyl)amino]-3-ethylphenylalanyl)amino]butoxy}-6-hydrox ybenzoate



Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS 30:CLASS 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:CLASS 20:CLASS 29:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 38:CLASS 39:CLASS 40:CLASS 47:CLASS 51:CLASS 52:CLASS 53:CLASS 54:CLASS 48:CLASS 49:CLASS 50:CLASS 56:CLASS

32-50 33-51 34-52

1-2 1-6 2-3 3-4 4-5 5-6 21-22 21-26 22-23 23-24 24-25 25-26 31-32 31-36 32-33 33-34 34-35 35-36 38-39 38-40

8-68 9-10 9-65 9-66 10-11 10-63 10-64 11-61

35-53

16-21 16-57 16-58 17-60 18-20 22-54 23-27 25-55

36-41

40-42

exact bonds :

normalized bonds:

1-2 1-6 2-3

1-70 2-69 4-43 6-71 8-9 8-67

11-62 12-47 13-15 15-16 15-59 26-56 27-28 27-48 27-49 30-38

57:CLASS 58:CLASS 59:CLASS 60:CLASS 61:CLASS 63:CLASS 64:CLASS 65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:CLASS 70:CLASS

2 L6

=> d 17 1-2 ibib abs hitstr

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS 2002:869580 CAPLUS

ACCESSION NUMBER:

DOCUMENT NUMBER: 137:353320

Preparation of amino(oxo) acetic acid derivatives as TITLE:

selective protein tyrosine phosphatase inhibitors Liu, Gang; Xin, Zhili; Pei, Zhonghua; Li, Xiaofeng;

Szczepankiewicz, Bruce G.; Janowick, David A.; Oost,

Thorsten K.

PATENT ASSIGNEE(S): USA

U.S. Pat. Appl. Publ., 60 pp., Cont.-in-part of U.S. SOURCE:

Pat. Appl. 2002 72,516.

CODEN: USXXCO

DOCUMENT TYPE:

LANGUAGE:

INVENTOR(S):

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO. DATE
US 2002169157	A1	20021114	US 2002-85157 20020227
US 2002035137	A1	20020321	US 2001-918928 20010731
US 2002072516	A1	20020613	US 2001-941471 20010829
PRIORITY APPLN. INFO.	:		US 2000-228651P P 20000829
			US 2000-650922 A2 20000829
			US 2001-918928 A2 20010731
			US 2001-941471 A2 20010829

OTHER SOURCE(S): MARPAT 137:353320

Compds. B-L-A-N(D) COCO2P2 [A are rings of defined structure; B = H, alkyl, aryl, arylalkyl, heterocyclyl, or heterocyclylalkyl; D = substituted Ph, alkyl, or 1-alkenyl [the substituent at the o- or 2-position is alkoxy, alkyl, sulfamoyl, amino, cyano, nitro, CO2P1, SO3H, P(O)(OH)2, CH2P(O)(OH)2, CHFP(O)(OH)2, CF2P(O)(OH)2, or C(:NH)NH2] or certain 5-membered heterocycles; P1, P2 = H, alkyl, alkenyl, arylalkyl, cycloalkyl, cycloalkylalkyl; L = (un)substituted (hetero)alkylene] or their therapeutically acceptable salts were prepd. as protein tyrosine kinase 1B (PTP1B) inhibitors. Thus, N-[5-[[N-acety1-4-[(carboxycarbonyl)(2-carboxyphenyl)amino]-3-ethylphenylalanyl]amino]pentan oyl]-L-methionine and Me 2-[4-[[N-acetyl-4-[(carboxycarbonyl)(2carboxyphenyl]amino]-3-ethylphenylalanyl)amino]butoxy]-6-hydroxybenzoate resp., for inhibition of PTP1B.

IT 436864-07-2P 436864-18-5P

> RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(prepn. of amino(oxo)acetic acid derivs. as selective protein tyrosine phosphatase inhibitors)

RN436864-07-2 CAPLUS

Benzoic acid, 2-[4-[[2-(acetylamino)-3-[4-[(carboxycarbonyl)(2-CNcarboxyphenyl)amino]-3-ethylphenyl]-1-oxopropyl]amino]butoxy]-6-hydroxy-, 1-methyl ester (9CI) (CA INDEX NAME)

RN436864-18-5 CAPLUS

CN

Benzoic acid, 2-[4-[[2-(acetylamino)-3-[4-[(carboxycarbonyl)(2carboxyphenyl)amino]-3-ethylphenyl]-1-oxopropyl]amino]butoxy]-6-hydroxy-(9CI) (CA INDEX NAME)

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 2002:450342 CAPLUS

137:33535

DOCUMENT NUMBER: TITLE:

Preparation of amino (oxo) acetic acids as selective

protein tyrosine phosphatase inhibitors

INVENTOR(S): Liu, Gang; Szczepankiewicz, Bruce G.; Pei, Zhonghua;

USA

Xin, Zhili; Janowick, David A.

PATENT ASSIGNEE(S): SOURCE:

U.S. Pat. Appl. Publ., 44 pp., Cont.-in-part of U.S.

Ser. No. 918,928.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
US 2002072516 US 2002035137 US 2002169157	A1 20020613 A1 20020321 A1 20021114		20010829
WO 2003020688 W: CA, JP,	A1 20030313	WO 2002-US24506	20020227
RW: AT, BE, LU, MC,	BG, CH, CY, CZ, DE, NL, PT, SE, SK, TR	DK, EE, ES, FI, FR,	GB, GR,

PRIORITY APPLN. INFO.: US 2000-228651P 20000829

US 2000-650922 A2 20000829 US 2001-918928 A2 20010731 IE, IT,

US 2001-941471 A2 20010829

OTHER SOURCE(S):

MARPAT 137:33535 Compds. B-L-A-N(D)COCO2P2 [A are rings of defined structure; B = H, alkyl, aryl, arylalkyl, heterocyclyl, or heterocyclylalkyl; D = substituted Ph, alkyl, or 1-alkenyl, in which the substituent at the o- or 2-position is alkoxy, alkyl, amino, cyano, nitro, CO2P1, SO3H, P(O)(OH)2, CH2P(O)(OH)2, CHFP(O)(OH)2, CF2P(O)(OH)2, C(:NH)NH2, or certain 5-membered heterocycles; P1, P2 = H, alkyl, alkenyl, arylalkyl, cycloalkyl, cycloalkylalkyl; L = (un) substituted (hetero) alkylene] or their therapeutically acceptable salts were prepd. as protein tyrosine kinase 1B (PTP1B) inhibitors. N-[5-[[N-acetyl-4-[(carboxycarbonyl)(2-carboxyphenyl)amino]-3ethylphenylalanyl]amino]pentanoyl]-L-methionine and Me

2-[4-[[N-acetyl-4-[(carbo arbonyl) (2-carboxyphenyl] amino] - ethylphenylalanyl) amino] butoxy]-6-hydroxybenzoate were prepd. and showed Kic = 0.077 .+-. 0.012 and 0.016 .+-. 0.003 .mu.M, resp., for inhibition of PTP1B.

436864-07-2P 436864-18-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of amino(oxo)acetic acids as selective protein tyrosine phosphatase inhibitors)

436864-07-2 CAPLUS

IT

RN

CN

CN

Benzoic acid, 2-[4-[[2-(acetylamino)-3-[4-[(carboxycarbonyl)(2carboxyphenyl)amino]-3-ethylphenyl]-1-oxopropyl]amino]butoxy]-6-hydroxy-, 1-methyl ester (9CI) (CA INDEX NAME)

RN 436864-18-5 CAPLUS

Benzoic acid, 2-[4-[[2-(acetylamino)-3-[4-[(carboxycarbonyl)(2-carboxyphenyl)amino]-3-ethylphenyl]-1-oxopropyl]amino]butoxy]-6-hydroxy-(9CI) (CA INDEX NAME)